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A Hill-series approach to wavefunction nodes

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Abstract

The Hill-series method is shown to have several advantages for treating the Schrödinger equation when the wavefunction obeys the Dirichlet boundary condition $\Psi(R) = 0$. A novel combination of the virial theorem, the Hill-series method and a finite difference method is used to find the node positions of the wavefunction for several excited states of perturbed oscillator and coulombic systems and to find critical radii for the hydrogen atom.

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1. Introduction

The Hill-series method was recently used in complex variable form to find the complex resonance energies for several systems [1]. In [1] it was also explained how the method can give bound state energies for both finite and infinite systems, using an approach which the present author developed some 20 years ago [2]. Fernandez referred to [1] when he showed that his Riccati–Padé method can calculate the same eigenvalues as the Hill-series method [3] but did not do so when he later showed that his method can be made to work for both finite and infinite systems [4]. In the present work, we show that the Hill-series approach offers several advantages in the treatment of finite systems for which potential used in the radial Schrödinger equation is a few-term polynomial. We proceed by means of an original application, the location of the node positions of an excited state wavefunction by an approach based on energy calculations. We show how the use of a simple auxiliary finite difference shooting procedure speeds up the task of finding accurate node positions.

Section 2 describes the relevant theory for the Hill-series approach. Section 3 explains how a simple finite difference scan can produce approximate node positions which are then refined by the Hill-series method. Section 4 gives some specimen results for perturbed oscillator systems. Section 5 explains the use of internal and external differentiation. Section 6 shows how the method can be extended to deal with coulombic systems so as to give the critical cage radii for the bounded hydrogen atom. Section 7 discusses several examples from the recent

literature to illustrate the accuracy of the method of the present work. Section 8 gives a brief conclusion.

2. The Hill-series method with internal differentiation

We review here the main features of the theory which are essential for the understanding of the original applications studied in the present work. As a specific illustrative example we will take the perturbed oscillator Hamiltonian

$$H = \alpha[-D^2 + L(L+1)r^{-2}] + V(1)r^2 + V(2)r^4 \quad (1)$$

and write the wavefunction for any desired state of angular momentum L in the form

$$\Psi(r) = \exp(-\beta r^2/2)r^{L+1} \sum A(J)r^{2J}. \quad (2)$$

Inserting the wavefunction from (2) into the Schrödinger equation $H\Psi = E\Psi$ and comparing coefficients gives the recurrence relation

$$\alpha(2J+2)(2J+2L+3)A(J+1) = [\alpha\beta(4J+2L+3) - E]A(J) + \sum U(K)A(J-K), \quad (3)$$

where $U(2) = V(2)$ and $U(1) = V(1) - \alpha\beta^2$.

We do not take the traditional step of inserting the coefficients $A(J)$ directly into (2) in order to work out the wavefunction at a specific radius R (so as to apply the Dirichlet condition $\Psi(R) = 0$). Instead, we suppose that we are going to use a given number of terms in the sum appearing in (2) and then factor out the term R^{2N} from the sum, giving for the sum of the terms up to R^{2N} the result

$$R^{2N}[A(N) + A(N-1)X^2 + \dots + A(0)X^{2N}], \quad (4)$$

where X is the reciprocal coordinate $X = 1/R$. We denote the sum in the square bracket by $F(N)$. Inspection of (4) shows that if we add the next term $A(N+1)R^{2N+2}$ to the sum (with a similar factorization) we obtain the recurrence relation

$$F(N+1) = X^2F(N) + A(N+1). \quad (5)$$

A study of the preceding equations reveals that at a fixed r value ($r = R$) it is sufficient to take the quantity $F(N)$ as representing the wavefunction, since all other factors are constant at that fixed r value. Thus we can concentrate on the task of making $F(N)$ zero as a function of the trial energy E , with the obvious empirical proviso that we should gradually increase N until any studied eigenvalue reaches a limiting value.

Since the coefficients $A(J)$ clearly depend on E and on the potential, we can take partial derivatives of them with respect to E and to $V(1)$. Denoting these derivatives by $AE(J)$ and $AV(J)$, respectively, direct inspection of the recurrence relation (3) shows at once that the $AE(J)$ and the $AV(J)$ also obey (3), with two very simple changes: a term $-A(J)$ is added on the right of the $AE(J)$ equation, and a term $A(J-1)$ is added on the right of the $AV(J)$ equation. Simultaneous propagation of the three sets (A, AE, AV) is thus easy, since all three recurrence relations involve the same coefficients. The starting condition is also very simple: all coefficients are set at zero, except for $A(0)$, which is set equal to 1. Differentiation also yields two obvious partner equations for (5), involving the pairs (FE, AE) and (FV, AV) . The only non-zero initial values in the whole set of coefficients are $F(0) = A(0) = 1$.

The recurrence relations are used up to some large N value and then the initial trial E is corrected by using the second-order Newton's method replacement (designated by an assignment statement)

$$E := E - F(N)/FE(N) \quad (6)$$

while the expectation value $\langle r^2 \rangle$ is found from the equation

$$\langle r^2 \rangle = -FV(N)/FE(N). \quad (7)$$

Setting $X = 0$ gives the Hill determinant method [5], which, as equation (5) shows, involves studying the individual coefficient $A(N + 1)$ rather than the sum of the series. Using a finite R with $X = 1/R$ gives results for the case in which the infinite barrier is placed at $r = R$. The use of (6) for finding energy values was outlined long ago for the special Hill determinant case $X = 0$ [6], while the use of (7) for the direct calculation of expectation values was developed in [7]. If the extra term on the right of the $AV(J)$ recurrence relation is $A(J - 2)$ instead of $A(J - 1)$ then we obtain the expectation value of x^4 rather than that of x^2 . Using $A(J - 3)$ would give the expectation value of x^6 , which can be formally regarded as being present (with a zero coefficient) in the potential.

It is important here to note some important computational details which help to give the method of this work both accuracy and flexibility. The first point refers to scaling. The coefficients $A(J)$ etc fall off rapidly in magnitude as N increases. It is thus useful to scale the quantities in the equations at each step, usually by dividing them all by the modulus of $A(J + 1)$. The only requirement is that the relative magnitudes of the important quantities are left unchanged, thus maintaining the correct ratios to be used in (6) and (7). Only the recurrence relation coefficients with indices from $J - 2$ to $J + 1$ need to be scaled (along with F , FE and FV), since they are the only ones needed for the next step. The calculation can if desired be carried out with only a small number of coefficients which are recycled as the calculation proceeds, although there is no problem in taking N up to several hundreds without the need for the use of such a compact form of the algorithm. The second computational point relates to the angular momentum variable, referred to by the standard symbol L in our equations. As will be shown later, the Hill-series method is applicable for any real value of L (not just the traditional physical quantized values). However, many computational languages reserve the symbol L for an integer variable. Thus to ensure the full range of applicability of the calculation a double precision variable such as XL should be used in the programmed version of (3) and its partner recurrence relations. The value of this procedure is shown by some examples in sections 5 and 6.

The third important computational point refers to the use of the Newton's method rootfinder formula (6). In the present work, we use a good preliminary finite difference locator for an initial trial energy and so do not have to move far to find the nearest eigenvalue. Even so, it is worthwhile to include a maximum shift parameter SHM in the computer program, to be used as follows. The nominal shift, $SH = -F(N)/FE(N)$ is first evaluated and is then divided by $[1 + \text{ABS}(SH/\text{SHM})]$ so as to keep its magnitude less than SHM. This cures a traditional defect of Newton's method; if by chance an initial guess for a root is near an extremum then the very small gradient in the denominator will give a large shift towards a distant root which is far from the desired nearest root.

3. Finding wavefunction nodes

If we set $X = 0$ in the equations then we obtain an eigenvalue E_0 for infinite space. If the associated wavefunction has a zero at $r = R_M$ then a calculation with $X = 1/R_M$ will give E_0 as one of the possible eigenvalues. Thus the technical problem is that of adjusting R so as to obtain E_0 as a calculated eigenvalue. Having found some excited state E_0 value we need a set of initial approximate node positions. Obtaining such a set is, of course, much faster than making many trial-and-error searches with the Hill-series method alone. Here a simple finite difference method produced by the present author in 1977 [8] turns out to be an ideal

auxiliary tool, since it works for any angular momentum and uses the raw potential $V(r)$ with the angular momentum term removed. If we use the fixed steplength h and introduce the ratio $W(r) = \Psi(r+h)/\Psi(r)$ the method of [8] leads to the simple recurrence relation

$$[r+h(L+1)]W(r) = [2+(h^2/\alpha)(V(r)-E)]r - [r-h(L+1)]/W(r-h). \quad (8)$$

Starting at $r = h(L+1)$ we see that the second term on the right vanishes and also $r+h(L+1)$ becomes exactly $2r$, giving the initial value for $W(L+1)$. We then proceed up to some upper limit of r appropriate for the state considered. Whenever W becomes negative we calculate $r+h/(1-W)$, which gives a linearly interpolated node position. The E value used is the E_0 from the Hill determinant ($X=0$) calculation. The finite difference equation is used only in a passive manner (with a single traverse) to produce approximate node positions. It is not used in the traditional active manner to calculate the energy. It will thus produce one extra unphysical node at a large r value, as the finite difference approximate wavefunction diverges up or down.

We now take the approximate R_M value for a node and use the Hill-series method with $X = 1/R_M$ to calculate $\langle r^2 \rangle$, $\langle r^4 \rangle$ and E (which is close to E_0). The virial theorem

$$4V(1)\langle r^2 \rangle + 6V(2)\langle r^4 \rangle - 2E = R dE/dR \quad (9)$$

then gives us dE/dR , so that the shift in the node position is found by calculating $(E_0 - E)/(dE/dR)$. After two or three repetitions of this process the calculated node position becomes stable to double precision and the calculated energy correctly equals the infinite space value E_0 . It is possible to calculate the expectation value appearing in (9) directly, by using $4V(1)A(J-1) + 6V(2)A(J-2)$ as the extra term on the right in the $AV(J)$ recurrence relation (and including $A(J-2)$ in the rescaling process).

4. Some numerical examples

One obvious check on the method of this paper is provided by the simple harmonic potential x^2 , since the wavefunction node positions are the zeros of an appropriate Hermite polynomial. There are also some previous results for the potential x^4 . In 2004, Nanayakkara [9] described an ingenious algebraic method which combined a Riccati equation approach with complex contour integration to calculate the node positions of the wavefunction for the one-dimensional Schrödinger equation. He gave a numerical demonstration of his method for the Hamiltonian $-D^2 + x^4$. We thus initially applied our method to these two simple cases. We should note that, although our method works for a radial equation (and thus employs the symbol r) the case of a one-dimensional state is treated simply by setting $L = 0$ for odd states and $L = -1$ for even states. For such problems the traditional symbol x is used in the literature; our occasional mixing of the symbols x and r when referring to other workers' results should not cause any problems. Table 1 shows some excited state results for the potentials x^2 and x^4 . The nodes for the x^2 case, as obtained by our method, are equal to double precision to the roots of the Hermite polynomial $H(6) = 8x^6 - 60x^4 + 90x^2 - 15$, as required for this excited state. Our results for the x^4 potential extend those of [9] to double precision. Both the Hill-series method and the finite difference scanning method of this work are adjusted to work with the basic interval from $r = 0$ up to some assigned maximum r value and can work with any given angular momentum. For example, they can work with $L = -1/2, 1/2$, etc, which would refer to a two-dimensional problem. Table 2 shows results for the potential $r^2 + r^4$ and for excited states of several different angular momenta, in order to demonstrate the flexibility of the method.

Table 1. Node positions for an excited state of the Hamiltonian $-D^2 + r^M$ for $M = 2$ and 4 and for $L = -1$. The node position predicted by the finite difference scanner is given in the initial bracket, followed by the extra digits added by the Hill-series method. The value of the gradient dE/dR is also given. The $M = 2$ values are given first. The E_0 values from the $X = 0$ calculation are 13 for $M = 2$ and 37.923 001 027 033 98 for $M = 4$. The parameter values used were $N = 100$ and $\beta = 1$ for $M = 2$, $\beta = 3$ for $M = 4$.

M	Node R value	$-dE/dR$
2	(0.4360)774 119 276 17	59.394 625 377 902
	(1.335)849 707 401 37	17.796 260 809 380
	(2.350)604 973 674 49	7.878 435 381 857
4	(0.2550)759 567 834 07	297.342 639 089 743
	(0.7657)747 417 472 26	98.619 326 592 853
	(1.2838)904 374 4813	56.728 904 560 258
	(1.840)620 422 758 08	33.815 177 479 343

Table 2. Node positions for some excited states of the radial Hamiltonian $-D^2 + r^2 + r^4$ and for three different values of angular momentum. The results are shown in the order $L = -1, -1/2, 0$. The $X = 0$ energies are (in order) 53.449 102 139 6653, 56.779 859 125 6604 and 34.640 848 321 1113. The parameters are $N = 100$, $\beta = 3$.

L	Node R value	$-dE/dR$
-1	(0.214)869 384 844 852	497.388 421 838 535
	(0.645)519 756 828 157	164.542 598 367 257
	(1.080)695 147 558 61	96.105 945 314 974
	(1.530)549 601 087 92	63.603 237 927 181
	(2.026)234 439 972 74	39.678 456 185 046
-1/2	(0.319)208 581 734 979	355.460 095 901 017
	(0.733)968 171 799 709	153.408 263 005 406
	(1.156)283 755 176 36	94.968 630 963 404
	(1.594)598 436 606 43	64.312 400 753 227
	(2.079)486 937 311 93	40.557 820 584 329
0	(0.534)466 750 077 262	128.919 500 503 147
	(1.077)055 890 601 29	61.620 286 740 841
	(1.658)895 929 408 39	34.231 205 940 092

Although the calculations are designed to produce energies and expectation values without the need to store an explicit wavefunction or to perform quadratures, it is still possible to obtain some detailed information about the wavefunction. We are, for example, obtaining accurate wavefunction node positions, but can go further. Starting from the Schrödinger equation it is possible to show that, for the case of a wavefunction normalized in the region 0 to R , with $\Psi(R) = 0$, the value of dE/dR exactly equals $-\alpha(d\Psi/dr)^2$ at $r = R$ (see [10] and the references therein). The finite difference scanner can give good estimates of the wavefunction extrema by indicating the r values at which $W(r)$ passes through the value 1. Modifying the Hill-series method to work for Neumann boundary conditions would involve a more complicated formalism but would, of course, permit accurate location of the extrema of the wavefunction.

5. Internal and external differentiation

We have applied our method to the results for a bounded oscillator given in two recent works [11, 12] and find general agreement, except that our method adds several digits of accuracy to the energies quoted in those works. We note that in [11] the expectation values of r^2 and r^4 were found by numerical quadrature, which requires the evaluation of the wavefunction at each r value and also the calculation of the normalization integral for the wavefunction. The approach of the present work is able to work out $\langle r^2 \rangle$ and $\langle r^4 \rangle$ without ever evaluating an explicit wavefunction. The case of the expectation value of r^{-2} , found by quadrature in [11], appears to present a more severe challenge for our approach but it also provides an example of the distinction between what we term internal and external differentiation.

We denote by internal differentiation the direct procedure described in section 3, which uses a differentiation process within the basic equations to give direct expectation values. If we recall that the full potential includes the term $\alpha L(L+1)r^{-2}$ then it is clearly possible in principle to perform a differentiation with respect to L . On noting that the coefficient $V(-2)$ takes the form $\alpha L(L+1)$ we arrive at the equation

$$dE/dL = \alpha(2L+1)\langle r^{-2} \rangle. \quad (10)$$

Inspection of the recurrence relation (3) shows that the variable L appears several times in the terms, so that internal differentiation will produce a more complicated form for the AV recurrence relation which has both $A(J)$ and $A(J+1)$ on the right. The process which we call external differentiation, on the other hand, involves the actual addition of a small increment $dV(K)$ to a potential coefficient $V(K)$, followed by a recalculation of the energy so as to obtain a finite difference numerical estimate of $\langle r^K \rangle$ by dividing the energy increment dE by $dV(K)$. The method of the present work has the remarkable feature that it works for any L value, not just for the traditional physical angular momentum values. Thus, for example, for a state with $L=0$ it is possible to set $L=0.000005$ and -0.000005 in turn and use the resulting energy change to obtain an accurate finite difference estimate of dE/dL , leading to a value for the expectation value of r^{-2} . For example, for the ground $L=0$ state of the Hamiltonian $(1/2)(-D^2 + r^2)$ we find at $R=2$ the energy 1.764816438780637 for $L=0$. Using the two L values given above produces the respective energies 1.764823178413304 and 1.764809699154426, leading to a value of 2.695851776 for $\langle r^{-2} \rangle$, in close agreement with the value found by detailed quadrature in [11].

6. General target energies: the hydrogen atom

Although the target energy E_0 used in the node calculation was the infinite space (Hill determinant) energy, it is clear that it could be any particular desired energy. As an example table 3 shows what the calculation gives if it is applied to the ground state ($L=-1$) wavefunction for the potential $r^2 + r^4$ so as to find the R value which would yield a desired eigenvalue. For small R values the particle in a box energy formula $E = \pi^2/(4R^2)$ gives a good initial estimate of the R value needed to produce a given energy.

As a further example, the double well Hamiltonian $-D^2 - r^2 + r^4$ has an infinite space ground state ($L=-1$) energy of about -0.308250 . Using the target energy zero gives an R value of 2.23990127322082, which is still well beyond the potential minimum at roughly 0.707.

The examples above dealt with oscillator systems but the target energy zero was also used in the critical radius calculations for the enclosed hydrogen atom [13], and it is obvious that the method of this work will be effective for such a calculation. To deal with the problem we

Table 3. The R values $R(E)$ needed to give a specified energy E for the groundstate ($L = -1$) of the Hamiltonian $-D^2 + r^2 + r^4$. The $X = 0$ energy is 1.392 351 641 530 292. The parameters are $N = 100$ and $\beta = 4$.

E	$R(E)$
2	1.190 204 707 126 25
3	0.929 143 152 091 552
4	0.795 258 657 019 837
5	0.707 851 045 167 367
6	0.644 574 461 510 190
7	0.595 902 064 976 313
8	0.556 909 334 969 012
9	0.524 738 990 300 515
10	0.497 597 395 889 723
15	0.405 884 284 185 298
20	0.351 388 007 302 600
30	0.286 839 597 719 898
40	0.248 390 228 451 412
50	0.222 158 699 106 960

use the same kinetic energy and angular momentum terms which appear in the Hamiltonian (1), with $\alpha = \frac{1}{2}$, but change the potential to be $-Z_0 r^{-1} + V(1)r$. The wavefunction is then taken in the form

$$\Psi(r) = \exp(-Zr)r^{L+1} \sum A(J)r^J. \quad (11)$$

Substituting this wavefunction into the Schrödinger equation leads to a recurrence relation for the $A(J)$:

$$\alpha(N+2)(N+2L+3)A(J+2) = [2Z\alpha(L+J+2) - Z_0]A(J+1) - (E + \alpha Z^2)A(J) + V(1)A(J-1). \quad (12)$$

This is the analogue of equation (3). The analogue of equation (5) is

$$F(N+1) = XF(N) + A(N+1) \quad (X = 1/R). \quad (13)$$

The virial equation for this case (the analogue of equation (9)) is

$$3V(1)\langle r \rangle - Z_0\langle r^{-1} \rangle - 2E = R dE/dR. \quad (14)$$

The quantities obtained by internal differentiation are introduced just as for the oscillator problem, except that a derivative $-d/dZ_0$ is needed in order to find $\langle r^{-1} \rangle$. The recurrence relation (12) and its partners are treated by starting at $J = -1$, with $A(0) = F(0) = 1$ as the only initial non-zero values.

As a test of the energy calculating capability of the method we have applied it to the confined hydrogen atom problems treated in some recent works [12, 14–16]. We obtained overall agreement with the results of those works, with several digits of extra accuracy. The calculation in [12] for the potential $-8/r + 4/r^2$ (with $L = 1$) is of particular interest, since it involves an unorthodox angular momentum value which is the positive root of the quadratic equation $L^2 + L - 10 = 0$. The Hill-series method can deal with this unorthodox L and yields for the first excited state the energy $-1.447\,656\,821\,925\,36$, which is more accurate than the value obtained in [12].

Table 4. Selected critical cage radii (the R values for which $E = 0$) for the hydrogenic Hamiltonian $-(1/2)D^2 - 1/r$. The initial values are taken from table 1 of [13] and are shown in a bracket, followed by the extra digits given by the Hill-series refining process. L is the angular momentum and n is the principal quantum number. A Z value of roughly $1/n$ suffices, with an N value of up to 300 to obtain convergence for the higher states.

(L,n)	R_C
0,1	(1.8352)463 302 6549
0,4	(12.937)431 736 8921
0,9	(105.46)478 098 7433
1,2	(5.0883)082 272 7504
1,5	(32.900)106 781 876
1,9	(104.46)159 310 9102
2,3	(9.617)366 041 705 914
2,7	(61.703)829 030 4546
3,4	(15.363)450 025 4520
3,8	(77.718)828 595 4322
4,5	(22.292)167 655 2037
4,8	(73.410)149 335 7275
5,6	(30.380)419 632 5576
5,9	(89.601)350 015 7361
6,7	(39.611)386 689 5650
6,9	(82.594)040 376 6115

When we return to the task of finding the nodes for an excited state wavefunction we can proceed in the same way as that used for the oscillator problems. The finite difference scanner works just as before, with the appropriate potential being used. We have tried a simple test calculation for the 3s state of the hydrogen atom, for which the wavefunction has a factor $(2r^3 - 18r^2 + 27r)$. The two non-zero nodes thus obey a quadratic equation. Our Hill-series method correctly gave the node positions $R = 1.901\,923\,788\,646\,68$ and $7.098\,076\,211\,353\,33$. For the critical radius calculation (with target energy zero) we followed the easy procedure of starting with the critical radii given in table 1 of [13]. Table 4 shows a selection of the results which were obtained, revealing how the present method increases the attainable accuracy.

The choice of parameters $Z_0 = 0$, $V(0) = 1$ allows us to treat the case of the Hamiltonian $-D^2 + r$, which was treated in [4]. Our method allows us to obtain accurate energies and expectation values for a wide range of values of R and L . However, [4] only dealt with the case $L = 0$, for infinite space and for $R = 1$, and quoted Riccati–Padé results of low accuracy for some excited states. For example, for the $n = 3$ state the calculations in [4] were only carried sufficiently far to give the energies 6.786 708 086 for infinite space and 158.411 for $R = 1$, while we quickly obtained the respective energies 6.786 708 090 071 76 and 158.413 789 814 309 by using the parameters $N = 100$ and $\beta = 6$ in the Hill-series method of this work. As the above numerical values indicate, the method of [4] seems to have more difficulty with the smaller R value. We found that in general the particle in a box formula $E = n^2\pi^2/R^2$ gives good initial energy estimates at $R = 1$. As an original contribution, more in keeping with the topic of this work, we show in table 5 the node positions for the wavefunction of the $n = 3$ state, which was the highest state studied in [4], both for the infinite system and for $R = 1$. The node positions at $R = 1$ are, as is physically reasonable, very close to those of the simple sine function wavefunction which is appropriate to a box containing a zero potential.

Table 5. Wavefunction nodes for an excited state of the Hamiltonian $-D^2 + r$ (for $L = 0$) which was treated in [4]. The nodes are given first for $R = 1$, corresponding to an energy value of 158.413 789 814 309, and then for infinite space, corresponding to an energy value of 6.786 708 090 071 76. An N value of 200 was used, with Z values varying between 3 and 6.

Node R value	$-dE/dR$
(0.249)703 473 748 430	1267.315 369 156 95
(0.499)604 214 519 874	632.656 894 810 74
(0.749)702 847 163 407	421.103 717 386 39
(1.266)148 261 976 21	9.233 603 432 221 59
(2.698)175 864 594 08	3.492 817 636 392 16
(4.448)600 679 611 99	1.454 928 413 312 04

Table 6. The function $\lambda(E)$ for the groundstate for the potential $x^6 + \lambda x^2$, with $\alpha = 1$ and angular momentum $L = -1$. The results of the Riccati–Padé method [17] are shown and the following bracket gives the extra digits obtained by the Hill-series method.

E	$\lambda(E)$
0.0	-3
0.2	-2.565 867 876(167938)
0.4	-2.098 071 121(005531)
0.6	-1.593 117 785(068834)
0.8	-1.047 382 878(08497)
1.0	-0.451 719 35(7)(6965098)
1.2	0.181 206 723(9)(8816911)
1.4	0.871 366 5843(314408)
1.6	1.616 770 801(495743)
1.8	2.420 669 59(1)(0918536)
2.0	3.286 052 010(32286)

7. Some further applications

The flexibility of the Hill-series method enables it to be modified to handle two further problems which have been treated in the modern literature. By adding an extra term $V(3)x^6$ to the potential in the Hamiltonian (1) we can treat the potential studied in [17], where the particular potential $x^6 + \lambda x^2$ was used, with the kinetic energy factor $\alpha = 1$. The work [17] studied the inverse problem of finding the λ value which would yield an assigned energy E for a selected state. To handle this problem by the methods of the present work does not even require the use of the virial theorem, since we have the direct result that $dE/d\lambda$ equals the expectation value of x^2 , which we obtain along with the energy. We can thus treat the problem for a range of L and R values. However, [17] only treated the infinite space case for the lowest two states in one dimension (corresponding to $L = 0$ and $L = 1$), comparing the $\lambda(E)$ values from an approximate perturbation approach with those found by using the Riccati–Padé method. For our numerical approach we obviously use the assignment statement

$$\lambda := \lambda - (E_0 - E)/\langle x^2 \rangle \tag{15}$$

to adjust the λ value so as to obtain the target energy E_0 . Table 6 shows our results for the groundstate with $L = -1$.

Table 7. The energy and the expectation value of r for the two-dimensional hydrogen atom (i.e. for $L = -1/2$) as a function of the radius R . The results for the present work appear in the second row for each R value. The last three digits of the $\langle r \rangle$ value from [19] are given after those from [18]. The energy from [18] is given in the first row.

R	E	$\langle r \rangle$
0.5	3.907 318 37	0.192 0880(533)(531)
	3.907 318 370 054 34	0.192 088 053 178 330
1.0	-1.349 785 72	0.336 8245(426)(420)
	-1.349 785 716 814 21	0.336 824 542 023 1443
2.0	-1.981 158 59	0.474 5295(650)(650)
	-1.981 158 591 165 108	0.474 529 565 056 930
4.0	-1.999 986 57	0.499 9085(584)(593)
	-1.999 986 566 533 668	0.499 908 559 351 00
8.0	-2.000 000 00	0.499 9999(888)(999)
	-1.999 999 999 996 86	0.499 999 999 906 49

The preceding example dealt with a perturbed oscillator problem but we now take a further example involving a confined two-dimensional hydrogen atom [18], so that we must now use the version of the Hill-series method which appeared in section 6. We have checked that our method can give all the results for varying values of angular momentum and R which appear in the tables of [18] and shall concentrate on the results in table 2 of [18], which show how the groundstate energy and expectation values depend on R . The calculations of [18] used a Numerov–Cooley finite difference method to find energies and wavefunctions, so that the expectation values of r and r^2 were found by quadrature using the calculated wavefunction. We should note here that the authors of [18] overlooked the use of Richardson extrapolation, which would have improved the accuracy of their eigenvalues with less computational effort; the principal energy error in their method varies as h^4 , where h is the steplength. The Hill-series approach gives the energies and the expectation values without any quadrature. Table 7 shows the groundstate energy of [17] as compared with those of our method and the $\langle r \rangle$ values of [18, 19] as compared with ours. Our accurate results show that the calculation of the work [19] is more accurate than that of [18] for the task of calculating $\langle r \rangle$.

8. Conclusion

The theory and the numerical results clearly demonstrate that the Hill-series method is not only more simple than that of [4] (which involves both Padé approximants and Hankel determinants) but also has the advantage of being able to work out expectation values as well as energies for both bounded and unbounded systems and for arbitrary angular momentum values. We have shown how this capability makes it possible to find wavefunction nodes and critical radii, and to use arbitrary target energies. The simple finite difference node predictor was also found to be highly accurate and so could be used together with any other method for the location of node positions. The methods of the present work have the computationally efficient (and amusing) feature that they can produce all the calculated quantities without needing to store an explicit wavefunction or to perform any quadratures. Several comments have been made in the text about the efficient programming of the equations, since most readers should be able to produce fairly speedily a computer program to implement the method of this work. The approach via

external differentiation treated in section 5 is independent of the particular Hill-series method and could be used as a supplement to most existing eigenvalue techniques in order to find expectation values. Indeed, a blend of internal and external differentiation has been used in conjunction with the Riccati–Padé method to treat oscillators with nonlinear self-interaction potentials [20]. The Riccati–Padé method does not involve a variable parameter such as the β of our method, although it can give rise to more than one possible energy for a state as the dimension of the Hankel determinant increases [4].

In the present work, parameters such as β and Z are used in order to control the rate of convergence of the calculated energies as N is increased. A change in β of 20% or so around our quoted values has negligible effect on the calculated energy but mainly changes the number of basis states needed to obtain full convergence of the energy. Thus the Hill-series approach gives results of acceptable accuracy when normal double precision is used. In an earlier work in this journal [21] the use of a non-zero β value for oscillator problems in the previous literature was criticized and it was shown that the use of the value $\beta = 0$ could lead to accurate energies for the quartically perturbed oscillator. It should be noted, however, that the criticism involved comparing older single precision calculations with calculations in [21] which used hundreds of digits of precision in order to perform an explicit summation of the series appearing in equation (2), which is avoided in the present work. More relevantly in the light of recent developments [1], it is precisely the presence of a non-zero β (changed to a complex variable) which makes it possible to extend the calculation to deal with resonances. Large numbers of digits of precision were also used in [22] to obtain very accurate eigenvalues for a range of potentials using the Frobenius method. For some calculations which are sensitive to the effects of rounding errors higher precision is a useful diagnostic tool, as the results of [22] show. However, the present author's view is that the currently increasing tendency to blast every calculation with hundreds of digits of precision might eventually have deleterious effects on the role played by subtlety and ingenuity in computational physics.

While revising this work the author has been made aware of a new research report [23] which applies the AIM approach to the problem of a confined hydrogen atom. Table 4 of [23] gives critical cage radii for the angular momentum values 0 and 1. Allowing for the different definition of n used in [23], the results of the new AIM calculation agree exactly with the results for $L = 0$ and 1 which we show in table 4 of the present work, which gives us further confidence in the numerical accuracy of our results.

The present work set out to show that the positions of wavefunction nodes can be found solely by means of energy calculations and dealt only with polynomial potentials, since the literature contains a plentiful supply of previous comparison energies for such potentials. However, one of our original works on the more traditional use of the Hill-series method [2] actually dealt with an exponential screened Coulomb potential, for which the potential is represented by a quickly convergent power series. The use of 10 or 20 terms in the potential series instead of 2 or 3 caused no essential difficulty for the method, except that it became necessary to perform an extra check on the convergence of the results as the number of potential terms used was increased. Thus the method should also be applicable (at least for sufficiently large R values) to the potential $x^2/(1 - x^2/R^2)^2$, which was treated by means of the AIM approach in a recent work [24].

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